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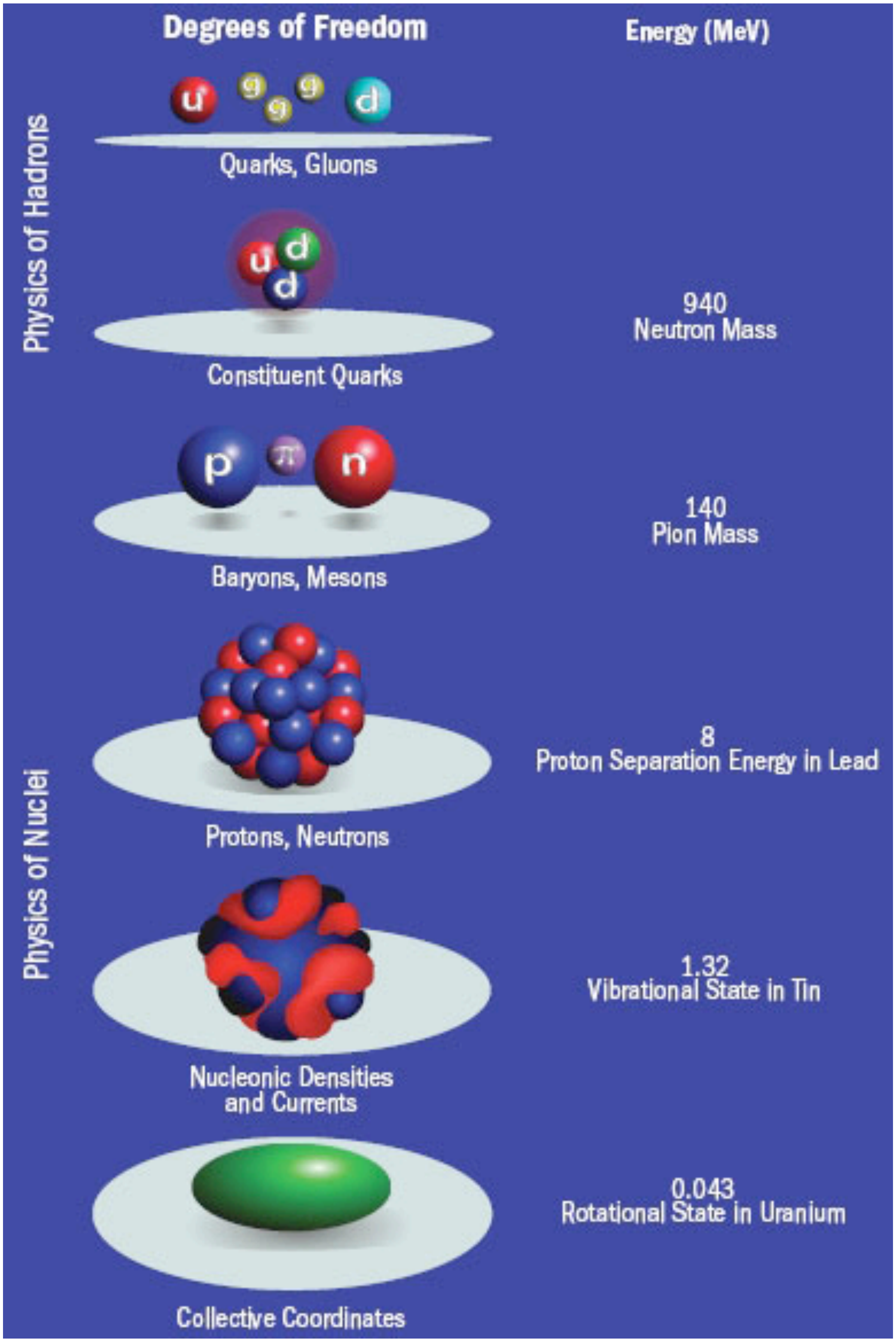
Universities and DOE National Laboratories join forces to understand the nucleus of an atom

(*Nanowerk News*) Nuclear physics is the study of the tiny, massive core of an atom, a complex micro-world of particles and forces. Nearly all the mass in the visible universe is locked away in atomic nuclei, as is nearly all the energy. The physics of the nucleus lies at the heart of element formation in exploding stars, as well as sources of energy for public use and national defense. Scientists strive for a comprehensive, unified description of all nuclei, a portrait of the nuclear landscape which incorporates all nuclear properties and forces in one framework. Such a model would allow for more accurate predictions of the nuclear reactions involved in all sorts of processes, from the creation of new elements to the improvement of nuclear reactors.

Around 50 researchers — theoretical physicists, computer scientists, and applied mathematicians — from nine U.S. universities, seven national laboratories, and research institutes across Europe and Japan, have come together in an effort to develop a more complete description of the atomic nucleus and its interactions. Their computational nuclear physics project, known as Universal Energy Density Functional (UNEDF), is led by Ewing Lusk (Argonne National Laboratory) and Witold Nazarewicz (University of Tennessee/Oak Ridge National Laboratory). The project is part of the U.S. Department of Energy's Scientific Discovery through Advanced Computing (SciDAC) program, funded by the Office of Science.

The UNEDF collaboration includes researchers from seven national laboratories and nine U.S. universities: Ames Laboratory, Argonne National Laboratory, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, Central Michigan University, Iowa State University, Michigan State University, Ohio State University, San Diego State University, the University of North Carolina, Texas A&M-Commerce, the University of Tennessee-Knoxville, and the University of Washington.

A nucleus is one of the most complicated environments in nature because all fundamental forces come into play. The four fundamental forces are called the strong force, electromagnetic force, weak force, and gravity. The constituents of a nucleus are protons and neutrons (collectively referred to as nucleons), which are themselves made of fundamental particles known as quarks and gluons. Each proton or neutron is made of three quarks, which are held together by the exchange of gluons. The quarks and gluons are governed by the strong force; their dynamics are responsible for the strong interaction between nucleons. In addition, both quarks and nucleons interact through the electromagnetic force. This is the familiar force through which particles with the same electric charge repel, and particles with opposite electric charges attract. The protons give each nucleus a net positive charge, so two nuclei will repel each other electromagnetically. Finally, the so-called "weak force" allows some of these particles to transform into others, which is the source of radioactivity. For instance, a neutron can transform into a proton by emitting an electron and a neutrino. While the force of gravity is insignificant inside the nucleus, it determines the existence of neutron stars — gigantic nuclei of stellar proportions. So a complete description of nuclear matter will have to incorporate the physics of all of these forces.



The basic elements (degrees of freedom) of strongly-interacting matter depend on the energy of the experimental probe and the distance scale. The building blocks of the theory of strong interactions, *quantum chromodynamics (QCD), are quarks and gluons. Hadrons (baryons and mesons) can often be described by the dynamics of the effective (or constituent) quarks, with the gluon degrees of freedom being integrated out. The classical nuclear physics problem is an effective approximation to QCD. It involves a strongly interacting quantum mechanical system of two fermionic species, protons and neutrons. A common starting point for nuclear physics is an inter-nucleon interaction, represented by a potential or by a set of meson-exchange forces. For complex nuclei, calculations involving all protons and neutrons become prohibitively difficult. Therefore, a critical challenge is to develop new approaches that identify the important degrees of freedom of the nuclear system and are practical in use. Such a strategy is similar to what is being used in other fields of science, in particular in condensed matter physics, atomic and molecular physics, and quantum chemistry. Of particular importance is the development of the energy density functional, which may lead to a comprehensive description of the properties of both finite nuclei and extended asymmetric nucleonic matter. Here, the main building blocks are the effective fields represented by local proton and neutron densities and currents. Finally, for certain classes of nuclear models, in particular those representing emergent many-body phenomena that happen on a much lower energy scale, the effective degrees of freedom are collective coordinates describing various vibrations and rotations and the large-amplitude motion as seen in fission.*

An improved description of the nuclear landscape will also require a better understanding of the nuclear "many-body problem" of many protons and neutrons mutually interacting through complex forces. The physics of many-body interactions can become quite complicated, so scientists turn to computers for help with the solutions. Thus, advancing the computational methods for modeling the nucleus is a major focus of this project. "The key objectives are maximal predictive power and well-quantified uncertainties" says Witold (Witek) Nazarewicz, co-director of the project.

One step toward completing a model for the nucleus is to find an "optimal energy density functional" for nuclei, a mathematical tool that can be used to compute the physics of all nuclei in the nuclear landscape. This important goal gives the project its name, Universal Energy Density Functional (UNEDF). Such a functional would allow scientists to compute important properties such as nuclear reaction rates and how much energy can come from a reaction. The tools developed by UNEDF enable predictions of nuclear properties that cannot be measured in nuclear laboratories, and allow the importance of future measurements to be assessed.

Recent achievements of the UNEDF collaboration include the state-of-the art computation of the charge distribution inside Carbon-12, which is a crucial test for theory; computation of short-lived nuclei Fluorine-14 and Fluorine-17, whose properties are important to processes in stars that cause elements to form; description of the "n+t reaction," a type of reaction that is important for understanding how the fuel is assembled in an implosion at the National Ignition Facility; derivation of the nuclear functional from interactions between protons and neutrons; advanced optimization of the nuclear functional; and massive calculations of various nuclear properties, including fission. To this end, the UNEDF scientists used the fastest supercomputers available for research.

The SciDAC team has made great strides towards meeting and in some cases exceeding the initial goals of the project, bringing the power of supercomputers to bear on complex theoretical problems. The computational approach has enabled the team to achieve a number of other important new results. To find out more about the UNEDF highlights, the team invites you to visit http://unedf.org/content/highlights_onepagers.phpExternal link.

Source: *Max Planck Institute of Quantum Optics*